

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.29 days

Global applicability domain: Outside

Local applicability domain index: 7.76e-02

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found

2-Methylhexane

Measured: 12.5

Predicted: 5.54

Image not found

2-Methylheptane

Measured: 12.5

Predicted: 3.99

Image not found

3-Methylhexane

Measured: 157

Predicted: 6.83

Image not found

2,4-Dimethylheptane

Measured: 61.9

Predicted: 4.29